Introduction to Mathematical Modelling (I002891)

Course size   *(nominal values; actual values may depend on programme)*

Credits 6.0   **Study time** 180 h

Course offerings in academic year 2024-2025

A (semester 2)   English   Gent

Lecturers in academic year 2024-2025

Van Liedekerke, Paul   LA26   lecturer-in-charge

Offered in the following programmes in 2024-2025	crdts	offering
Master of Science in Pharmaceutical Engineering	6	A

Teaching languages

English

Keywords

Calculus, differential equations, uncertainty quantification, dynamic system analysis

Position of the course

This course provides a basis for the formulation and usage of mathematical models necessary for simulations of pharmaceutical processes. These models heavily draw on differential equations and concepts from calculus.
In the first part the students are acquainted with basic mathematical techniques and methods that are required to understand, analyse and describe various production processes. Such a mathematical background is needed in preparation for building and simulation of process models. Subsequently, students are familiarized with systems of differential equations and (non-)linear differential equations, and introduced to analytical and numerical solution methods to be able to predict processes
In the second part of the course, students will learn how to deal with modeling uncertainty and probability.
In the third part, the students will learn how to perform a sensitiviy analysis and parameter estimation of the models, as well as how to decide how "good" a model is.

Contents

1. Functions of one variable: continuity, derivatives, Taylor series, Integration
2. Linearization of functions, root finding
4. Vectors and Matrices, eigenvalues, singular value decomposition
5. Functions of several variables: derivatives, Taylor series, gradient, Hessian
7. Introduction to differential equations
8. Qualitative analysis of 1st order diff eqns
9. Solving 1st order diff eqns numerically
10. Systems of diff eqns and higher order diff eqns
11. Laplace transformations
12. Mass balance equations and diffusion effects
13. Probabilistic modeling and stochastic simulations
14. Sensitivity analysis
15. Parameter estimation, Model evaluation, Model selection

Initial competences

Knowledge of basic mathematics : derivatives, integrals, matrix algebra, vectors. Basic knowledge of Python programming language is highly recommended.

Final competences

1 To understand the mathematical and geometric meaning of functions of one and more variables
2 To understand the mathematica land geometric meaning of polar coordinates, parametric functions, vector functions and vector fields.
3 To be able to use functions of multiple variables, polar coordinates, parametric functions, vector functions and vector fields
4 To build, follow and execute correct reasoning for functions of one and more variables.
5 To be able to work with functions of one and more variables in a correct and mathematically precise manner.
6 To be able to recognise diverse types of differential equations.
7 To be able to apply analytical solution techniques.
8 To be able to execute qualitative analyses of (sets of) differential equations.

9 To be able to use numerical solution methods for differential equations in pyhton.
10 To be able to translate a system description into a mathematical model as a set of differential equations
11 Be able to make the link between model results and physical reality.

12 Quantify and compare the sensitivity of model attributes.
13 Conduct a parameter estimation and quantify its reliability.

Conditions for credit contract

Access to this course unit via a credit contract is determined after successful competences assessment

Conditions for exam contract

This course unit cannot be taken via an exam contract

Teaching methods

Seminar, Lecture, Independent work

Extra information on the teaching methods

Theory in plenary lectures, exercises in PC-practicals

Study material

None

References

Adams, R.A. and Essex, C. Calculus 9th edition (2009). Pearson
P. Vanrolleghem & D. Dochain Bioprocess Model Identification. In: Advanced Instrumentation, Data Interpretation and Control of Biotechnological Processes. Eds. Van Impe J., Vanrolleghem P., Iserentant D., Kluwer (1998).

B.A. Oggunaike & W.H. Ray Process Dynamics, Modeling and Control. Oxford University Press (1994). L. Ljung System Identification - Theory for the User. Prentice-Hall (1999).

Trench, W.F., Elementary differential equations, Brooks/Cole Thomson Learning, 2001;
Boyce, W.E., DiPrima, R.C., Meade, D.B., Elementary Differential Equations and Boundary Value Problems, Wiley, 2017.

Course content-related study coaching

Study coaching is offered before and after each of the oral lectures and practicum or after appointment. There is also a forum on Ufora

Assessment moments

end-of-term assessment

Examination methods in case of periodic assessment during the first examination period

Written assessment with multiple-choice questions, Written assessment

Examination methods in case of periodic assessment during the second examination period

Written assessment with multiple-choice questions, Written assessment

Examination methods in case of permanent assessment

Presentation, Assignment

Possibilities of retake in case of permanent assessment

examination during the second examination period is not possible

Extra information on the examination methods

--- Klik om te editeren ---

Open book exam
solving problems on computer

Calculation of the examination mark

Periodic evaluation (exam) 70% - Permanent evaluation 30%
There is no second chance for the permanent evaluation.